

Esol (pretrained)

GPR

GPT-InChI

GPT-SMILES

GPT-SELFIES

Weave

GraphConv

TabPFN

accuracy

F<sub>1</sub> macro

F<sub>1</sub> micro

$\kappa$

0.4

0.2

0.4

0.2

0.4

0.2

0.4

0.2

0.0

10

15

20

25

30

35

40

45

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